

Single-hole dynamics in the t - J model

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The quasi-particle weight of a single hole in an antiferromagnetic background is studied in the semiclassical approximation. We start from the t - J model, generalize it to arbitrary spin S by employing an appropriate coherent state representation for the hole, and derive an effective action for the dynamics in the long-wavelength low-energy limit. In the same limit, we find an expression for the single-hole Green's function which we evaluate in an $1/S$ expansion. Our approach has the advantage of being applicable in one *and* in two dimensions. We find two qualitatively different results in these two cases: while in one dimension our results are compatible with a vanishing quasi-particle weight, this weight is found to be finite in two dimensions, indicating normal quasi-particle behavior of the hole in this last case.

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I. INTRODUCTION

Although more than 30 years have elapsed since Brinkman and Rice¹ published their pioneering work on the propagation of a hole in a quantum antiferromagnet, this subject still attracts a lot of attention. Central to this problem is the question whether the motion of a hole in a strongly correlated system is coherent or not, i.e., whether the hole can be considered as a quasi-particle in the sense of Landau's Fermi-liquid theory, or whether, as was first suggested by Anderson^{2,3}, it is more appropriate to view the hole as a constituent particle of a Luttinger-like liquid. For a long time, the interest in this question has been fueled by the expectation that an accurate description of the hole dynamics in a strongly correlated electron system would be the crucial first step towards an understanding of the physics of the cuprate superconductors. More recently, this interest has been revived, since the dynamics of holes in one- (1D) and two-dimensional (2D) antiferromagnets has become experimentally accessible in angle-resolved photoemission spectroscopy (ARPES)^{4,5}. The key quantity that can in principle be obtained from the results of ARPES is the spectral weight Z at the ground state energy E_G of the systems. A nonvanishing spectral weight, $Z \neq 0$, implies that the hole is a quasi-particle, e.g., a spin-polaron consisting of the bare hole with a spin polarisation cloud around it. On the contrary, a vanishing Z signals that the hole causes a global rearrangement of the original ground state such that the exact single-hole wave function becomes orthogonal to the wave function of a bare hole in the antiferromagnetic ground state. ARPES data for the one-dimensional copper oxide chain compound SrCuO₂, see Ref. 5, and for the two-dimensional layered compound Sr₂CuO₂Cl₂, see Ref. 4, show that the hole dynamics differ significantly between the 1D and the 2D case (see the discussion in Ref. 5). The features of the spectra of the 1D compound fit rather well with the concept of spin-charge separation that has emerged from Bethe-Ansatz and bosonization studies of the 1D Hubbard model^{6,7,8} and from the exact solution of the t - J model at the supersymmetric point^{9,10}. Theoretically, spin-charge separation implies that for long wavelengths, the Hamiltonian of a hole can

be decomposed into two commuting parts, $H = H_h + H_s$, where both the holon part H_h and the spinon part H_s , are free-fermion Hamiltonians^{9,10,11}. As a consequence, the single-hole Green's function takes the form

$$G(p, \tau) = \int \frac{dQ}{2\pi} G_h(p - Q, \tau) Z(Q, \tau). \quad (1)$$

Here, $G_h(k, \tau)$ is the propagator of a free holon, whereas the function $Z(Q, \tau)$ is entirely determined by the spinon dynamics; Q is the spinon momentum. While the holon Green's function G_h is a free-fermion propagator indeed, $\text{Im } G_h(k, \omega) = \pi\delta(\omega - \varepsilon_h(k))$ with $\varepsilon_h(k)$ the holon kinetic energy, the spinon contribution $Z(Q, \tau)$ is a highly nontrivial singular function. Technically, this last feature has its origin in the fact that the original hole operator $c_{i\sigma}$ does not simply factorize into a holon and a spinon operator, $c_{i\sigma} \neq h_i^\dagger s_i$. Rather, in the representation of $c_{i\sigma}$ by h_i^\dagger and s_i , an additional phase factor $\exp(i\theta_s)$ is needed, where the phase θ_s depends on the spinon operators s_j only. This phase factor accounts for the *phase-string* effect^{11,12,13}: as the physical hole moves through the (quasi)-ordered spin background, it trails a string of overturned spins behind it. Using the *phase-string* picture, Suzuura and Nagaosa¹¹ have obtained a qualitatively correct result for the single-hole spectral function in 1D. We note, however, that Sorella and Parola^{9,10} have derived their detailed results for the spinon function $Z(Q, \tau)$ in 1D without making use of a *phase-string* picture. Thus in 1D, the different approaches lead to the same conclusion: there is spin-charge separation in this case, and the hole Green's function shows Luttinger-liquid-like behavior. A recent quantum Monte-Carlo (QMC) simulation of the single-hole dynamics in the one-dimensional t - J model has confirmed these results¹⁴. In two dimensions, the situation is less clear. Many studies of the hole dynamics in the two-dimensional t - J model have been based on an effective Hamiltonian which describes the hole as a spinless fermion that is coupled linearly to the magnon excitations of the antiferromagnetic background. In obtaining the hole Green's function, the coupling between the hole and the magnons is then treated in the self-consistent Born approximation (SCBA), and a normal quasi-particle

peak is found in the single-hole spectral function^{15,16,17,18,19}. It must be emphasized that the SCBA is a perturbative method so that the quasi-particle picture is inherent in this method. However, a finite quasi-particle weight of a hole has also been found in a non-perturbative large-spin study of the 2D t-J model²⁰. Moreover, a recent QMC simulation²¹ lends support to these results in a wide range of the model parameter J/t and of the momentum k of the propagating hole. But, remarkably, two theoretical predictions by Sorella²² concerning the behavior of the quasi-particle weight $Z(Q)$ for $J/t = 2$ at the antiferromagnetic wave vector $\mathbf{Q} = (\pi, \pi)$ are less well confirmed by the simulations in Ref. 21. Apart from this seemingly minor discrepancy between QMC simulation and certain theoretical predictions, there is further work which casts doubt on the validity of the quasi-particle picture for a hole in the two-dimensional t -J model: results from a high temperature series expansion for the momentum distribution of the particles in the t -J model show a violation of Luttinger's theorem²³. This means that the ground state of the 2D t -J model is not connected adiabatically to the ground state of the noninteracting model as would be the case for a normal Fermi-liquid consisting of quasi-particles. More directly, it is claimed by Weng *et al.*^{12,13,24} that the phase-string picture, which explains the vanishing of the quasi-particle weight in 1D, applies in 2D too and has the same effect there. Despite this apparent failure of the quasi-particle picture, these authors suggest in Ref. 24 that the spectral features seen in ARPES can be explained satisfactorily in the framework of the t -J model by their theory. However, in a very recent QMC study Mishchenko *et al.*²⁵ contradict this suggestion, as they confirm the quasi-particle picture already found by Brunner *et al.*²¹.

In view of these contradictions between numerical and analytic analyses, we propose a new analytic approach to the calculation of the quasi-particle weight Z of a single hole in the t -J model. Our method has the advantage of being applicable in arbitrary space dimensions and is thus suitable to detect differences between the 1D and the 2D case. In 1D, our results are compatible with a power-law decay of the weight Z as the system size L increases to infinity, $Z \sim L^{-2X}$. On the contrary in 2D, this weight remains finite in the thermodynamic limit indicating that the quasi-particle picture is valid in this case.

The paper is organised as follows: Section II contains the derivation of the effective action of a single-hole in an antiferromagnetic background with the method of coherent states²⁶. In the later parts of the paper, we wish to employ a semiclassical expansion, i.e., an expansion in powers of the inverse spin length $1/S$. For this reason, we generalise the conventional t -J model in which every lattice site is either occupied by a spin $\frac{1}{2}$ particle or empty, to the case where the lattice sites are occupied either by an object with arbitrary but fixed spin S (particle) or by an object with spin $S - \frac{1}{2}$ (hole)²⁷. We implement this modification by an appropriate choice of the coherent-state representation for the particles which at the same time satisfies explicitly the constraint of forbidden double occupancy. In describing the local coupling of the hole to the spin degrees of freedom, it turns out to be crucial to use

local $SU(2)$ fields as the basic variables of the effective action instead of working with the local sublattice magnetization. In Section III, we employ the effective action of Section II to obtain a path-integral representation for the single-hole Green's function. Our aim is to extract from this function an expression for the quasi-particle weight Z of the hole which exhibits explicitly the dependence of Z on the system parameters, in particular its dependence on the linear system size L . To achieve this goal, we have to take recourse to the semi-classical expansion. In Section IV, we present and discuss our final results. Technicalities of the developments in Sections II and III are deferred to Appendices A and B.

II. PATH-INTEGRAL REPRESENTATION

In this Section, we derive an effective action for the motion of a single hole in an antiferromagnet. The underlying Hamiltonian is that of the t -J model,

$$\begin{aligned} \mathcal{H} = & -t \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{P} (c_{\mathbf{r}, \sigma}^\dagger c_{\mathbf{r}', \sigma} + h.c.) \hat{P} \\ & + J \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \hat{\mathbf{S}}_{\mathbf{r}} \cdot \hat{\mathbf{S}}_{\mathbf{r}'} . \end{aligned} \quad (2)$$

Here $c_{\mathbf{r}, \sigma}^\dagger$ and $c_{\mathbf{r}, \sigma}$ are the creation and annihilation operators for fermion states at site \mathbf{r} with spin projection σ , and $\hat{\mathbf{S}}_{\mathbf{r}} = \frac{1}{2} c_{\mathbf{r}, \alpha}^\dagger \boldsymbol{\sigma}_{\alpha, \beta} c_{\mathbf{r}, \beta}$ is the spin of the fermion. \hat{P} projects onto states where each lattice site is either empty or singly occupied. $\langle \mathbf{r}, \mathbf{r}' \rangle$ denotes nearest neighbor sites on a hypercubic lattice with lattice constant a in D dimensions. The main difficulty in analysing the properties of (2) lies in the strong interactions induced by the exclusion of doubly occupied sites. We deal with this difficulty by using an appropriate set of coherent states (cf. Refs. 28, 26) which takes these constraints into account explicitly. This leads to the following path-integral representation of the partition function \mathcal{Z} :

$$\mathcal{Z} = \int \mathcal{D}[\omega] e^{- \int_0^{\beta} d\tau \{ \langle \omega | \partial_\tau | \omega \rangle + \langle \omega | \mathcal{H} | \omega \rangle \}} . \quad (3)$$

The coherent states $|\omega\rangle$ are introduced and discussed in the Appendix A. They are parameterized by two fields; the anti-commuting fields $\eta_{\mathbf{r}}, \eta_{\mathbf{r}}^*$ which describe the hole, and the commuting field $g_{\mathbf{r}} \in SU(2)$ which determines the orientation of the spin (see Eq. (6) below). As is detailed in the Appendix, our coherent states are constructed such that they allow us to generalise to arbitrary spin S : Each lattice site is occupied either by an object with spin S (particle) or an object with spin $S - \frac{1}{2}$ (hole)²⁷. Then, the hopping term t in Eq. (2) exchanges spin S objects and spin $S - \frac{1}{2}$ objects on neighbouring lattice sites. The corresponding matrix elements are worked out in the Appendix A. In the parametrisation by η and g , the term entering the kinetic part of the action in Eq. (3) takes the form

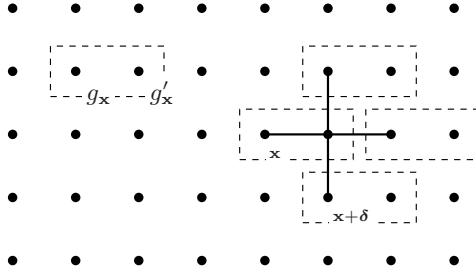


FIG. 1: Partitioning of the square lattice into plaquettes

$$\langle \omega | \partial_\tau | \omega \rangle = \sum_{\mathbf{r}} \left\{ (2S - \eta_{\mathbf{r}}^* \eta_{\mathbf{r}}) (g_{\mathbf{r}}^\dagger \partial_\tau g_{\mathbf{r}})_{\uparrow\uparrow} + \eta_{\mathbf{r}}^* \partial_\tau \eta_{\mathbf{r}} \right\}, \quad (4)$$

while in the Hamiltonian part

$$\begin{aligned} \langle \omega | \mathcal{H} | \omega \rangle &= \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle} \left\{ 2S t \left[\eta_{\mathbf{r}}^* \eta_{\mathbf{r}'} (g_{\mathbf{r}'}^\dagger g_{\mathbf{r}})_{\uparrow\uparrow} + (\mathbf{r} \leftrightarrow \mathbf{r}') \right] \right. \\ &\quad \left. + \frac{J}{4} (2S - \eta_{\mathbf{r}}^* \eta_{\mathbf{r}}) (2S - \eta_{\mathbf{r}'}^* \eta_{\mathbf{r}'}) \mathbf{n}_{\mathbf{r}} \cdot \mathbf{n}_{\mathbf{r}'} \right\}. \end{aligned} \quad (5)$$

In the case $S = \frac{1}{2}$, everything reduces to the ordinary t - J model. The unit vector

$$\mathbf{n}_{\mathbf{r}} = \frac{1}{2} \text{Tr} \{ \boldsymbol{\sigma} g_{\mathbf{r}} \sigma_z g_{\mathbf{r}}^\dagger \} \quad (6)$$

which occurs in the Heisenberg term in Eq. 5 points in the direction of the expectation value of the spin. The magnitude of the spin is S , or $S - \frac{1}{2}$, depending on the presence of a hole which is expressed by the occupation number $\eta_{\mathbf{r}}^* \eta_{\mathbf{r}}$. The amplitude of the hopping term $\eta_{\mathbf{r}}^* \eta_{\mathbf{r}'}$ in Eq. (5) is modulated by the actual state of the background spin, and this constitutes the main coupling between the hole- and the spin-subsystems. Note that, while the Heisenberg part depends on $g_{\mathbf{r}}$ only through the bilinear term (6), the $SU(2)$ -fields $g_{\mathbf{r}}$ at the individual lattice sites are needed to express the hopping term (see the related discussion of symmetries of the action in Ref. 29).

Proceeding towards the derivation of an effective action, we now divide the lattice into plaquettes each of which contains a pair of neighbouring sites of the two sublattices. We label these with \mathbf{x} , the lattice points of the A-sublattice. Then, the plaquette \mathbf{x} contains the fields $g_{\mathbf{x}}$ and $g'_{\mathbf{x}} \equiv g_{\mathbf{r}+a\hat{e}_x}$, on the A- and B-site, respectively, see Fig. 1.

In the conventional description of a two-sublattice antiferromagnet, one would introduce now the magnetisation $\mathbf{M} = \mathbf{S}_A + \mathbf{S}_B$ and the sublattice magnetisation $\mathbf{N} = \mathbf{S}_A - \mathbf{S}_B$ of each plaquette as new fields and integrate subsequently over \mathbf{M} .

In our $SU(2)$ description, we introduce the $SU(2)$ -field

$$M_{\mathbf{x}} := g_{\mathbf{x}}'^\dagger g_{\mathbf{x}}; \quad (7)$$

we choose the $SU(2)$ fields $g_{\mathbf{x}}$ and $M_{\mathbf{x}}$ as our new variables and, finally, we will integrate over the fields $M_{\mathbf{x}}$. A useful parametrization of M in terms of three real variables α , $\Re u$, and $\Im u$ is

$$M = \begin{pmatrix} e^{i\alpha} & 0 \\ 0 & e^{-i\alpha} \end{pmatrix} \begin{pmatrix} u & i \\ i & u^* \end{pmatrix} / \sqrt{1 + |u|^2} \quad (8)$$

(here, the label \mathbf{x} has been suppressed). Then, for an arbitrary phase α , the point $u = 0$ corresponds to the antiferromagnetic alignment of the spins within the plaquette, since

$$\begin{aligned} \mathbf{n}_{\mathbf{x}} \cdot \mathbf{n}'_{\mathbf{x}} &= \frac{1}{2} \text{Tr} \{ M_{\mathbf{x}}^\dagger \sigma_z M_{\mathbf{x}} \sigma_z \} \\ &= -1 + 2|u_{\mathbf{x}}|^2 + \mathcal{O}(u_{\mathbf{x}}^4). \end{aligned} \quad (9)$$

Next, we express all terms in the action by $M_{\mathbf{x}}$ and $g_{\mathbf{x}}$; we start with the Hamiltonian part. The vector between nearest neighbor plaquettes is denoted by $\delta = 2a\hat{e}_x, a\hat{e}_x \pm a\hat{e}_y, \dots$ (or 0), see Fig. 1. Then, the hopping term between two plaquettes in Eq. (5) contains the expression

$$g_{\mathbf{x}}'^\dagger g_{\mathbf{x}+\delta} = M_{\mathbf{x}} g_{\mathbf{x}}^\dagger g_{\mathbf{x}+\delta}. \quad (10)$$

Since we are aiming at a gradient expansion of the $SU(2)$ fields in the Hamiltonian part of the action, we replace $g_{\mathbf{x}}'^\dagger g_{\mathbf{x}+\delta}$ in the hopping term in Eq. (5) by

$$g_{\mathbf{x}}'^\dagger g_{\mathbf{x}+\delta} =: 1 + i\delta \cdot \mathbf{A}_{\mathbf{x}}, \quad (11)$$

where $\mathbf{A}_{\mathbf{x}}$ becomes the spatial derivative

$$\mathbf{A}_{\mathbf{x}} = -i g_{\mathbf{x}}^\dagger \nabla g_{\mathbf{x}}. \quad (12)$$

in the continuum limit. The Heisenberg term in Eq. (5) can also be conveniently expressed by $M_{\mathbf{x}}$ and $\mathbf{A}_{\mathbf{x}}$:

$$\begin{aligned} &\mathbf{n}_{\mathbf{x}+\delta} \cdot \mathbf{n}'_{\mathbf{x}} \\ &= \frac{1}{2} \text{Tr} \{ g_{\mathbf{x}+\delta}^\dagger g_{\mathbf{x}}' \sigma_z g_{\mathbf{x}}'^\dagger g_{\mathbf{x}+\delta} \sigma_z \} \\ &= \frac{1}{2} \text{Tr} \{ [1 + i\delta \cdot \mathbf{A}_{\mathbf{x}}]^\dagger M_{\mathbf{x}}^\dagger \sigma_z M_{\mathbf{x}} [1 + i\delta \cdot \mathbf{A}_{\mathbf{x}}] \sigma_z \} \end{aligned} \quad (13)$$

In the term entering the kinetic part of the action, Eq. (4), we introduce the time derivative

$$A_{\mathbf{x}}^\tau := -i g_{\mathbf{x}}^\dagger \partial_\tau g_{\mathbf{x}}. \quad (14)$$

Then, we have on the B-sites,

$$g_x'^\dagger \partial_\tau g_x' = M_x i A_x^\tau M_x^\dagger + M_x \partial_\tau M_x^\dagger. \quad (15)$$

Next, we collect all terms and expand the expressions in the exponent of the functional integral for \mathcal{Z} , Eq. (3), up to the second order in u_x . Finally, we perform the Gaussian integration over u_x and identify the effective action $\mathcal{A} = \int_0^\beta d\tau \mathcal{L}$ as the exponent in the resulting path-integral. The remaining integration fields are defined on the A-sublattice: on each plaquette there is one commuting field $g_x \in SU(2)$ for the remaining spin-degrees of freedom, and there are two anti-commuting fields η_x and $\tilde{\eta}_x = e^{i\alpha_x} \eta_{r+a\hat{e}_x}$ on each plaquette which describe the holes. Note that the phase α_x has been absorbed in the redefinition of the hole field on the B-sublattice; it disappears from the effective action. We work in the leading order in the gradients, A_x and A_x^τ so that the effective Lagrangian \mathcal{L} is accurate in second order in these gradients. \mathcal{L} can now be written as a sum of terms, each representing the contribution of a fixed number of holes. We retain only the zero- and one-hole contributions: $\mathcal{L} = -2\mathcal{N}DJS^2 + \mathcal{L}_{nl\sigma m} + \mathcal{L}_{1\text{-hole}} + \dots$. The first term is the energy of the classical antiferromagnetic state of a system with \mathcal{N} plaquettes. The fluctuations of the spins in the absence of holes are governed in the continuum limit by the well-known non-linear σ -model for the unit vector \mathbf{n}_x

$$\begin{aligned} \mathcal{L}_{nl\sigma m} = & \int \frac{d^D x}{2a^D} \left[\frac{1}{4DJ} \dot{\mathbf{n}}_x^2 + JS^2 a^2 \sum_{j=1}^D (\partial_j \mathbf{n}_x)^2 \right] \\ & + i \frac{S}{2} \int \frac{d^D x}{a^{(D-1)}} \mathbf{n}_x \cdot \dot{\mathbf{n}}_x \times \partial_1 \mathbf{n}_x \end{aligned} \quad (16)$$

The first two terms in Eq. (16) are temporal and spatial fluctuations, respectively ($\dot{\mathbf{n}}_x \equiv \partial_\tau \mathbf{n}_x$). The last term is the famous topological term which yields a zero mass for the fluctuations for half-integer spins in one dimension; for $D > 1$, this term is not effective (see, e.g., the discussion in Ref. 30). We wish to emphasise that we obtain here exactly the same result, Eq. (16), as in the conventional approach in which one uses the magnetisation $\mathbf{M} = \mathbf{S}_A + \mathbf{S}_B$ and the sublattice magnetisation as $\mathbf{N} = \mathbf{S}_A - \mathbf{S}_B$ as plaquette variables and then integrates over \mathbf{M} . However, our approach which uses the $SU(2)$ -fields g_x as basic variables turns out to be superior when the steps leading to $\mathcal{L}_{nl\sigma m}$ have to be performed for the hopping term of Eq. (5). From the procedure described above, we get

$$\begin{aligned} \mathcal{L}_{1\text{-hole}} = & \sum_x \left[\eta_x^* (\partial_\tau - i A_x^\tau \uparrow\uparrow) \eta_x + \tilde{\eta}_x^* (\partial_\tau - i A_x^\tau \downarrow\downarrow) \tilde{\eta}_x \right] \\ & + \sum_x \left[\eta_x^* h_x^{aa} \eta_x + \tilde{\eta}_x^* h_x^{bb} \tilde{\eta}_x \right] \\ & + \sum_{x,\delta} \left[\eta_{x+\delta}^* h_{x+\delta,x}^{ab} \tilde{\eta}_x + \tilde{\eta}_x^* h_{x,x+\delta}^{ba} \eta_{x+\delta} \right] \end{aligned} \quad (17)$$

where $h_{...}^{\alpha\beta}$ are the matrix elements of the effective Hamiltonian for the hole in the background of the g_x -fields. The diagonal elements are expressed in terms of the vector \mathbf{n}_x (bilinear in g_x^\dagger and g_x , see Eq. (6)) as follows

$$\begin{aligned} h_x^{aa} &= DJS + \frac{1}{8DJS} \dot{\mathbf{n}}_x^2 - \frac{JS}{16D} \sum_{\delta,\delta'} (\mathbf{n}_{x+\delta} - \mathbf{n}_{x+\delta'})^2 \\ h_x^{bb} &= DJS - \frac{1}{8DJS} \dot{\mathbf{n}}_x^2 - \frac{JS}{16D} \sum_{\delta,\delta'} (\mathbf{n}_{x+\delta} - \mathbf{n}_{x+\delta'})^2 \\ &- i \frac{1}{2} \mathbf{n}_x \cdot \dot{\mathbf{n}}_x \times \frac{1}{2D} \sum_{\delta} (\mathbf{n}_{x+\delta} - \mathbf{n}_x). \end{aligned} \quad (18)$$

The off-diagonal elements describe hopping from the A-sublattice to the B-sublattice and vice versa. They can only be expressed with the aid of the $SU(2)$ -field g_x itself:

$$\begin{aligned} h_{x+\delta,x}^{ab} &= \frac{-it}{DJ} \left[g_x^\dagger \partial_\tau g_x + JS \sum_{\delta'} \left(g_{x+\delta}^\dagger - g_{x+\delta'}^\dagger \right) g_x \right]_{\downarrow\uparrow} \\ h_{x,x+\delta}^{ba} &= \frac{it}{DJ} \left[g_x^\dagger \partial_\tau g_x + JS \sum_{\delta'} g_x^\dagger (g_{x+\delta} - g_{x+\delta'}) \right]_{\uparrow\downarrow}. \end{aligned} \quad (19)$$

The preceding equations complete the derivation of the effective action for a hole in the background of the spin-fields g_x . The approximations made so far were (i) the Gaussian integration over the variables u_x which describe the deviation from the antiferromagnetic order within a plaquette and (ii) the gradient expansion in temporal and spatial derivatives. Thus, the Euler angles defining the fields g_x should be smooth in space and time, but there is no limitation on their variation over large distances in space or time.

We remark that our effective one-hole Lagrangian, Eq. (17), differs significantly from the effective Lagrangian that has been derived by Shankar in Ref. 31,32 for the same physical situation. Partially, the difference stems from the fact that the work in Ref. 31,32 is based on a generalised t - J model which includes besides nearest neighbour (intersublattice) hopping also next-nearest neighbour (intrasublattice) hopping. Furthermore, however, terms that describe intersublattice hopping, i.e., the terms in the last line of Eq. (17), are neglected

in Ref. 31,32. It is argued that intersublattice hopping processes are necessarily accompanied by spin fluctuations and are therefore suppressed in a situation with strong short-range antiferromagnetic order. In our case of a t - J model with purely nearest neighbour hopping, the neglect of the corresponding terms in the effective Lagrangian would leave us with a static hole which is clearly not an appropriate description of the physical situation which we intend to consider.

III. GREEN'S FUNCTION

In order to obtain the quasi-particle weight Z of a hole in an antiferromagnetic background, we study the Green's function of a single hole in the t - J model

$$G_{\sigma,\sigma'}(\mathbf{r} - \mathbf{r}'; \tau) = \langle c_{\mathbf{r},\sigma}^\dagger(\tau) c_{\mathbf{r}',\sigma'}(0) \rangle \quad (20)$$

As is seen from the spectral representation, one can extract the quasi-particle weight from G in the limit of large imaginary time τ at zero temperature:

$$\begin{aligned} G_{\sigma,\sigma'}(0; \tau \rightarrow \infty) &\Big|_{T=0} \\ &\sim \frac{1}{L^d} \sum_{\mathbf{q}} e^{-(E_{\mathbf{q}}^{tJ} - E_0^{Heis.})\tau} |{}_{tJ}\langle \mathbf{q} | c_{\mathbf{q}\sigma} | 0 \rangle_{Heis.}|^2. \end{aligned} \quad (21)$$

Here, $|\mathbf{q}\rangle_{tJ}$ denotes the ground state of a single hole with momentum \mathbf{q} in the t - J model, $|0\rangle_{Heis.}$ the ground state of the Heisenberg model, and $E_{\mathbf{q}}^{tJ}$ and $E_0^{Heis.}$ the corresponding energies; L is the linear size of the system and d its dimension. The last factor in (21) represents the quasi-particle weight, and we are interested, in particular, in its size dependence. Our treatment of the Green's function is based on a path-integral representation for $G_{\sigma,\sigma'}(0; \tau)$. As in the previous Section, we generalise our considerations to arbitrary spin S and use the representation (A10) of the Fermion operators as a product of a Grassmann variable and an $SU(2)$ -matrix. Noting that $G_{\sigma,\sigma'}$ is diagonal in the spin-indices, $G_{\sigma,\sigma'}(0; \tau) =: \delta_{\sigma,\sigma'} S G(\tau)$, we arrive at the representation

$$\begin{aligned} G(\tau) = \frac{1}{Z} \int \mathcal{D}[\omega] \eta_{\mathbf{r}}(\tau) \eta_{\mathbf{r}}^*(0) [g_{\mathbf{r}}^\dagger(\tau) g_{\mathbf{r}}(0)]_{\uparrow\uparrow} \\ e^{-\int_0^\beta d\tau \{\langle \omega | \partial_\tau | \omega \rangle + \langle \omega | \mathcal{H} | \omega \rangle\}}. \end{aligned} \quad (22)$$

G is independent of \mathbf{r} , so that we can choose $\mathbf{r} = 0$ which we consider as the origin of the A-sublattice. Following the steps that led to the effective action in Section II, we decompose the lattice into plaquettes and integrate over the $SU(2)$ -field M_x which is defined within each plaquette. Next, we restrict the effective Lagrangian to zero-hole and one-hole terms, $\mathcal{L}_{nl\sigma m} + \mathcal{L}_{1-hole}$, see above. Performing then the integration over the Grassmann variables $\eta_{\mathbf{r}}$ and $\eta_{\mathbf{r}}^*$, we finally

arrive at the formal result

$$G(\tau) = \frac{\int \mathcal{D}[g] G^{1-hole}[g; \tau] [g_0^\dagger(\tau) g_0(0)]_{\uparrow\uparrow} e^{-\int_0^\beta d\tau \mathcal{L}_{nl\sigma m}}}{\int \mathcal{D}[g] e^{-\int_0^\beta d\tau \mathcal{L}_{nl\sigma m}}}. \quad (23)$$

Here, G^{1-hole} is the $\mathbf{r} = \mathbf{r}' = 0$ element of the hole Green's function in matrix representation, calculated for a fixed configuration of the $SU(2)$ -field g that describes the spins,

$$G^{1-hole}[g; \tau] = \left[T \left\{ e^{-\int_0^\tau d\tau' \mathbf{h}[g]} \right\} \right]_{00}. \quad (24)$$

This expression results as the solution of the corresponding equation of motion. T is the time ordering symbol and $\mathbf{h}[g]$ is defined as the matrix (on the spatial lattice) which connects the Grassmann variables η^* , $\tilde{\eta}^*$ and η , $\tilde{\eta}$ in the quadratic form in \mathcal{L}_{1-hole} , cf. Eq. (17). In the derivation of $G(\tau)$, Eq. (23), we have restricted not only the action but also the integration over the Grassmann variables to zero-hole and one-hole terms; in addition, we consider only the leading order in the limit $T \rightarrow 0$. Effectively, this implies the omission of any correction proportional to the fugacity of the hole, $e^{-DJS/T}$; here, DJS is the creation energy of one hole in a perfect antiferromagnetic background, cf. Eq. (18).

The general result for the Green's function, $G(\tau)$, Eqs. (23, 24), for one hole in the t - J model is valid under the conditions stated in connection with the derivation of the effective action, cf. the text after Eq. (19): in other words, it is valid whenever there is local antiferromagnetic order with a sufficiently large correlation length so that lattice effects play no role.

Hole- and spin- degrees of freedom are coupled in $G(\tau)$, because the hole Green's function $G^{1-hole}[g; \tau]$ depends on the time- and spatial fluctuations of the spin configuration, cf. Eqs. (18, 19). A further evaluation of $G(\tau)$ in the presence of this coupling would require the exact calculation of $G^{1-hole}[g; \tau]$ for each individual configuration of the $SU(2)$ background field $g_x(\tau)$. This is an impracticable task. Therefore, to be able to proceed we have to take recourse to approximations.

We start from the expression Eq. (23) for $G(\tau)$. In the limit $\tau \rightarrow \infty$, $G(\tau)$ has the spectral representation (cf. Eq. (21))

$$G(\tau \rightarrow \infty) \sim \frac{1}{N} \sum_{\mathbf{q}} e^{-E_{\mathbf{q}}(S)\tau} Z_{\mathbf{q}}(S), \quad (25)$$

where $E_{\mathbf{q}}(S)$ and $Z_{\mathbf{q}}(S)$ are the hole energy and the quasi-particle weight of the hole, respectively.

If we neglect the fluctuations of the spin configuration completely in Eq. (23), $g_x(\tau) = const.$, Eqs. (24, 18) yield $G^{1-hole}[g = const.; \tau] = e^{-DJS\tau}$, and $E_{\mathbf{q}}(S) = DJS$ and $Z_{\mathbf{q}}(S) = 1$ in this case. If we would neglect merely the coupling to the spin fluctuations in G^{1-hole} , we would obtain a non-trivial result for $Z_{\mathbf{q}}(S)$. In this case, the factorization of the hole- and the spin-part of $G(\tau)$ are reminiscent of the spinon-holon decomposition observed in one dimension.

The amplitudes of the spin fluctuations are controlled by the parameter $1/S$. In the sequel, we shall study the Green's function $G(\tau \rightarrow \infty)$, Eq. (25), in an expansion in powers of this parameter, i.e., in the semiclassical expansion:

$E_{\mathbf{q}}(S) = DJS + \mathcal{O}(S^0)$, $Z_{\mathbf{q}}(S) = 1 + \mathcal{O}(S^{-1})$. The technical details of this expansion are presented in the Appendix B. We are interested in the quasi-particle weight only. Therefore, we disregard all corrections to the hole energy beyond the lowest order. This is achieved by scaling $\tau = \tilde{\tau}/S$ and neglecting all terms proportional to powers of $\tilde{\tau}$ which would result from corrections to the lowest order of $E_{\mathbf{q}}(S)$ in Eq. (25) in a systematic expansion in $1/S$. Then, our procedure yields an average of just the quasi-particle weight over the Brillouin zone:

$$Z(S) = \frac{1}{N} \sum_{\mathbf{q}} Z_{\mathbf{q}}(S) = 1 - \frac{1}{S} Z^{(1)} - \frac{1}{S^2} Z^{(2)} + \mathcal{O}\left(\frac{1}{S^3}\right). \quad (26)$$

The fact that we cannot resolve the \mathbf{q} -dependence of the quasi-particle weight within an $1/S$ expansion, is easy to understand: as it is shown in the Appendix B, the expansion in $1/S$ also implies an expansion in the hopping amplitude t . Without hopping, $h^{ab} = h^{ba} = 0$ in Eq. (17), $\mathcal{L}_{\text{1-hole}}$ becomes local in the hole fields, and thus, the hole energy $E_{\mathbf{q}}(S)$ in Eq. (25) becomes dispersionless in leading order in the $1/S$ expansion so that we arrive at the average.

Our explicit results for the first two coefficients $Z^{(1,2)}$ of the $1/S$ expansion of the quasi-particle weight in one and two dimensions will be presented next.

IV. RESULTS AND SUMMARY

We start with the discussion of the one-dimensional case. The k -sums in the results for $Z^{(1,2)}$, Eqs. (B7, B8) in the Appendix B, are performed as integrals over the Brillouin zone with a cutoff at small momenta, $k \gtrsim k_0 = 2\pi/L$. Then, $Z^{(1)}$ diverges logarithmically with the system size L :

$$Z^{(1)} = \left(1 + \frac{4t^2}{J^2}\right) \frac{1}{2\pi} \ln \frac{L}{a}. \quad (27)$$

Here, we have neglected terms which remain finite in the limit $L \rightarrow \infty$ since they depend on the choice of the cutoff. For $S = 1/2$, the quasi-particle weight Z of a single hole is known to vanish algebraically with increasing system size L , $Z \sim L^{-2X}$ (see Refs. 9, 10). This behavior of Z reflects Anderson's orthogonality catastrophe^{33,34}: the states $c_{\mathbf{q}\sigma}|0\rangle_{\text{Heis}}$ and $|\mathbf{q}\rangle_{tJ}$ (see Eq. (21)), i.e., the bare one-hole state and the true one-hole eigenstate of the t - J model, are orthogonal in the thermodynamic limit. The orthogonality catastrophe is an effect of the quantum fluctuations, and therefore, it should not occur in the classical limit $S \rightarrow \infty$. Consequently, we expect that $\lim_{S \rightarrow \infty} X = 0$. This suggests that the expansion in Eq. (26) should be reformulated as an expansion of $\ln Z(S)$ in powers of $1/S$. Then, we get in first order for the exponent X the result $X = (1 + 4t^2/J^2)/(4\pi S)$.

At first, this looks quite satisfactory: the exact value for $S = 1/2$ at $t = 0$ is $X = 3/16$ (see Ref. 10). As t increases from zero, X also increases. This tendency is compatible with another exactly known result: at the supersymmetric

point $J/t = 2$, where the t - J model is exactly solvable, one finds value $X^{\text{Susy}} = 1/4$; see Ref. 9.

However when we try to improve the lowest order result by including the next order

$$Z^{(2)} = \left(\frac{1}{4} - \frac{4t^2}{J^2}\right) \left(\frac{1}{2\pi} \ln \frac{L}{a}\right)^2 + \mathcal{O}\left(\ln \frac{L}{a}\right), \quad (28)$$

we find in leading logarithmic order

$$\ln Z(S) = -\left(1 + \frac{4t^2}{J^2}\right) \frac{1}{2\pi S} \ln \frac{L}{4a} - \frac{3}{4} \left(\frac{1}{2\pi S} \ln \frac{L}{4a}\right)^2. \quad (29)$$

Here we have omitted a term of the order of $\frac{1}{S^2}(t/J)^4$, since it does not change the picture qualitatively. Obviously, this expression for $\ln Z(S)$ cannot simply be interpreted as the first two terms of an expansion in powers of $1/S$ of the exponent $X(S)$ in a power law $Z(S) \sim L^{-2X(S)}$. At first glance, one might think that the deviation from such an expansion can be attributed to the fact that in Eq. (26), the quantity $Z(S)$ is an average over the Brillouin zone of the quasi-particle weights $Z_q(S)$ so that one cannot expect to find a power-law dependence of $Z(S)$ on the system size L . However, for $t = 0$, i.e. for a static hole, for which $Z_q(S)$ is independent of the wave number q , Eq. (29) can still not be interpreted as an expansion in powers of $1/S$. The infrared divergent terms in $Z(S)$ show that instead of a straightforward expansion a renormalization group treatment is necessary. This is quite plausible, since $1/S$ is the coupling constant of the non-linear σ -model $\mathcal{L}_{\text{nl}\sigma m}$, Eq. (16), on which our $1/S$ expansion is based. However, in Eq. (23) the parameter $1/S$ appears not only as the coupling constant of σ -model $\mathcal{L}_{\text{nl}\sigma m}$, it also occurs in the hole Green's function, Eq. (24). Therefore, the standard renormalisation group procedure for the non-linear σ -model³⁵ cannot be applied in the present case. The development of an appropriate procedure is beyond the scope of this paper. Notwithstanding these complications, Eq. (29) shows a behavior compatible with a vanishing quasi-particle weight in one dimension.

In two dimensions, our general expressions Eqs. (B7, B8) for $Z^{(1,2)}$ yield a different picture: the k -sums converge at small momentum k . Thus, in contrast to the one-dimensional case, the average quasi-particle weight $Z(S)$ is independent of the system size. This means that up to the order $1/S^2$ of our large- S expansion there is no sign of an orthogonality catastrophe in the two-dimensional model. In recent, very elaborate numerical studies of t - J model on the square lattice^{21,25} it has been found that within this model, the spectral function of a single hole shows the signature of a coherent quasi-particle, i.e., the quasi-particle weight $Z_q(S)$ has been found to remain finite throughout the Brillouin zone. Although the semiclassical expansion does not allow us to determine the weights $Z_q(S)$ at individual \mathbf{q} points, our result for the average weight $Z(S)$ is consistent with these numerical findings.

In summary, in this paper we have presented a new approach to the problem of hole dynamics in the t - J model. We use

a generalisation of this model, which has originally been designed for spin $\frac{1}{2}$ particles, to describe particles with arbitrary spin S . This has allowed us to consider the case of large S in which the semiclassical approximation is applicable. This approximation has the advantage that it works independent of the spatial dimension of the system we wish to investigate. Therefore, we have been able to study the single-hole dynamics in one and in two dimensions on the same footing. In agreement with most previous investigations of the dynamical properties of a hole in the t - J model, we find a qualitative difference between these properties in one and in two dimensions: while in two dimensions the results of our $1/S$ expansion are compatible with the picture of the hole as a coherent quasi-particle in the sense of Landau's Fermi liquid theory, the hole appears to have a vanishing quasi-particle weight in the one dimensional case so that the quasi-particle picture fails in this case.

APPENDIX A: COHERENT STATES

We use the method of coherent states (for a recent review see Ref. 28) in order to deal with the problem of excluded double occupancy²⁶. First, consider the case of spin $1/2$. Then, the Hilbert space consists of a fermionic state with spin up $c_{\uparrow}^{\dagger}|0\rangle$, a fermionic state with spin down $c_{\downarrow}^{\dagger}|0\rangle$, and a hole $|0\rangle$ at each lattice site. Following Ref. 29, we introduce (at each lattice site) the states

$$\begin{aligned} |\omega\rangle &= e^{[\eta c - c^{\dagger}\eta^*]} c^{\dagger} |0\rangle \\ &= (1 - \frac{1}{2}\eta^*\eta) c^{\dagger} |0\rangle + \eta |0\rangle \end{aligned} \quad (\text{A1})$$

with

$$c^{\dagger} = c_{\uparrow}^{\dagger} g_{\uparrow\uparrow} + c_{\downarrow}^{\dagger} g_{\downarrow\uparrow}. \quad (\text{A2})$$

Here, the parameters η, η^* are Grassmann variables and describe the hole. g is a $SU(2)$ -matrix, $g^{\dagger}g = \mathbb{1}_2$; it can be parametrized by three Euler angles and describes the orientation of the spin. In this Appendix, we index a unit matrix with its dimension.

Next, we generalize the coherent states $|\omega\rangle$ to the case of arbitrary spin S . Then, the Hilbert space consists of $(2S+1) + 2S$ states at each lattice site which are the states of a spin S , $|S, m = -S \cdots S\rangle$ and a spin $S - \frac{1}{2}$, $|S - \frac{1}{2}, m = -(S - \frac{1}{2}) \cdots (S - \frac{1}{2})\rangle$. Now define, cf. Ref. 27,

$$|\omega\rangle = (1 - \frac{1}{2}\eta^*\eta) R |S, S\rangle + \eta R |(S - \frac{1}{2}), (S - \frac{1}{2})\rangle. \quad (\text{A3})$$

Here, the rotation matrix R can be represented for arbitrary spin in the following way by three Euler angles ψ, θ , and ϕ

$$R = e^{-i\phi\hat{S}^z} e^{-i\theta\hat{S}^y} e^{-i\psi\hat{S}^z}. \quad (\text{A4})$$

Instead of using the Euler angles, one can also parametrize R by the elements of the $SU(2)$ -matrix g which is the $S = \frac{1}{2}$

representation of R . In this paper, we use g as the fundamental variable. In the case $S = \frac{1}{2}$, (A3) coincides with (A1). For the application of the method of coherent states, we need to specify the expectation values of the operators in the Hamiltonian with the states $|\omega\rangle$. Obviously, $\langle\omega|\omega\rangle = 1$. The spin operator \hat{S} acts as usual on the spin-states; with $s = S$ or $s = S - \frac{1}{2}$:

$$\langle s, s | R^{\dagger} \hat{S} R | s, s \rangle = s \mathbf{n}. \quad (\text{A5})$$

In terms of g , the unit vector \mathbf{n} reads

$$\mathbf{n} = \frac{1}{2} \text{Tr} \{ \sigma g \sigma g^{\dagger} \}. \quad (\text{A6})$$

For the expectation value of the spin with $|\omega\rangle$, we find

$$\langle\omega|\hat{S}|\omega\rangle = \frac{1}{2} (2S - \eta^*\eta) \mathbf{n}. \quad (\text{A7})$$

The Fermion operators c_{σ} (we use $\sigma = \uparrow, \downarrow \equiv \pm 1$) link the states with spin S and $S - \frac{1}{2}$,

$$c_{\sigma} |S, m\rangle = \gamma_{\sigma, m} |S - \frac{1}{2}, m - \sigma \frac{1}{2}\rangle. \quad (\text{A8})$$

Here, $\gamma_{1,-S} = \gamma_{-1,S} = 0$ and the remaining coefficients $\gamma_{\sigma, m}$ are uniquely determined by demanding that the relation between the Fermion operators and the spin is as in the case of $S = \frac{1}{2}$,

$$\frac{1}{2} (c_{\uparrow}^{\dagger}c_{\uparrow} - c_{\downarrow}^{\dagger}c_{\downarrow}) = \hat{S}^z \text{ and } c_{\uparrow}^{\dagger}c_{\downarrow} = \hat{S}^+. \quad (\text{A9})$$

We get

$$\langle\omega|c_{\sigma}|\omega\rangle = \sqrt{2S} \eta^* g_{\sigma\uparrow}. \quad (\text{A10})$$

The resolution of unity reads in our case

$$\int d\omega |\omega\rangle\langle\omega| = \mathbb{1}_{4S+1}. \quad (\text{A11})$$

The integration measure is

$$\int d\omega \dots = \int dg \int d\eta^* d\eta 2S e^{-\frac{1}{2S}\eta^*\eta} \dots. \quad (\text{A12})$$

Our convention $\int dg = 1$ for the invariant measure of g leads to

$$\int dg R |s, s\rangle\langle s, s| R^{\dagger} = \frac{1}{2s+1} \mathbb{1}_{2s+1}. \quad (\text{A13})$$

With the aid of Eqs. (A3,A12,A13), one quickly confirms that the dimension of the Hilbert space comes out correctly:

$$\begin{aligned} \text{Tr} \left\{ \int d\omega |\omega\rangle\langle\omega| \right\} \\ = \int d\eta^* d\eta 2S e^{-\frac{1}{2S}\eta^*\eta} (1 - 2\eta^*\eta) = 4S+1. \end{aligned} \quad (\text{A14})$$

To complete the list of relations involving the coherent states, we quote the expression entering the kinetic part of the action (we consider now ω to depend on τ)

$$\langle \omega | \partial_\tau | \omega \rangle = (2S - \eta^* \eta) (g^\dagger \partial_\tau g)_{\uparrow\uparrow} + \eta^* \partial_\tau \eta - \frac{1}{2} \partial_\tau (\eta^* \eta) \quad (\text{A15})$$

In deriving Eq. (A15), we used

$$\langle s, s | R^\dagger \partial_\tau R | s, s \rangle = 2s (g^\dagger \partial_\tau g)_{\uparrow\uparrow} . \quad (\text{A16})$$

APPENDIX B: $1/S$ EXPANSION

Here, we describe the simultaneous expansion of $G(\tau)$, Eq. (23), in the fluctuation amplitudes and in the hopping integral t . The antiferromagnetically ordered state, $\mathbf{n}_x(\tau) = \hat{e}_z$ is given by $g_x(\tau) = 1$ (cf. Eq. (6)). Then, it is convenient to characterize an arbitrary state by

$$g_x(\tau) = e^{i\sigma\epsilon(x,\tau)} e^{i\sigma_z\epsilon_z(x,\tau)} , \quad (\text{B1})$$

where we parameterize the field $g_x(\tau)$ by a $SU(2)/U(1)$ -symmetric part and a $U(1)$ -factor.

It is easily seen that the latter disappears from our considerations: $\mathbf{n}_x(\tau)$ is determined only by the two fields in the vector $\epsilon = (\epsilon_x, \epsilon_y)$ which enter the $SU(2)/U(1)$ -part of the field g ; the $U(1)$ -part, the last factor in (B1) drops out. Thus, the $U(1)$ -factor also drops out of $\mathcal{L}_{\text{nl}\sigma m}$. It still appears in $\mathcal{L}_{\text{1-hole}}$, Eq. (17), through the field

$$A_{x\sigma\sigma}^\tau(\tau) = \sigma \partial_\tau \epsilon_z(x, \tau) - i \left[e^{-i\sigma\epsilon(x,\tau)} \partial_\tau e^{i\sigma\epsilon(x,\tau)} \right]_{\sigma\sigma} \quad (\text{B2})$$

and through the off-diagonal matrix elements $h_{x+\delta,x}^{ab}$ and $h_{x,x+\delta}^{ba}$ (cf. Eq. (19)) in which the $U(1)$ -terms occur as the first and the last factor. Looking at Eq. (17) one recognises, however, that these $U(1)$ factors can be absorbed into the Grassmann fields by the gauge transformation

$$\eta_x(\tau) \rightarrow e^{i\epsilon_z(x,\tau)} \eta_x(\tau) , \quad \tilde{\eta}_x(\tau) \rightarrow e^{-i\epsilon_z(x,\tau)} \tilde{\eta}_x(\tau) , \quad (\text{B3})$$

so that they disappear from the integrands in the numerator and in the denominator on the r. h. s. of Eq. (23). Furthermore, in the integration measure ϵ_z and ϵ separate, $d\eta \propto d\epsilon_z d^2\epsilon \sin(2\epsilon)/\epsilon$, so that the integrations over ϵ_z cancel between the numerator and the denominator of the r. h. s. of Eq. (23). These considerations show that the field ϵ_z disappears completely from the expression Eq. (23) for the Green's function $G(\tau)$.

Now, we consider this expression in a systematic expansion with respect to ϵ , i.e. we expand on the r. h. s. of Eq. (23) the integration measure, the factors $G^{\text{1-hole}}$ and $[g_0^\dagger g_0]_{\uparrow\uparrow}$ in the integrand, and $\mathcal{L}_{\text{nl}\sigma m}$ in powers of ϵ . Inspection of the quadratic part of $\mathcal{L}_{\text{nl}\sigma m}$ shows that in this expansion, each additional power of ϵ beyond the second order yields an additional power of $1/\sqrt{S}$. We make this explicit by scaling the spin wave amplitude ϵ by a factor of $(4S)^{-1/2}$, $\epsilon = \tilde{\epsilon}/(4S)^{1/2}$ and the imaginary time by a factor of $(2dJS)^{-1}$, $\tau = \tilde{\tau}/(2dJS)$.

Then, the quadratic part in the new fields becomes independent of S and the spin wave dispersion reads

$$\omega_{\mathbf{k}} = \sqrt{1 - \gamma_{\mathbf{k}}^2} , \text{ with } \gamma_{\mathbf{k}} = \frac{1}{d} \sum_{s=1}^d \cos(k_s a) . \quad (\text{B4})$$

Relative to the leading order in S , $G(\tau) = \exp(-\tilde{\tau}/2)$, we want to obtain corrections up to and including the order $1/S^2$ accurately. Therefore, we retain terms up to the order $\tilde{\epsilon}^4$ in the factors $G^{\text{1-hole}}$ and $[g_0^\dagger g_0]_{\uparrow\uparrow}$ in the integrand, anharmonicities up to the order $\tilde{\epsilon}^4$ in $\mathcal{L}_{\text{nl}\sigma m}$, and terms up to the order $\tilde{\epsilon}^2$ in the measure (note that after the scaling, the measure already contains a prefactor of $1/S$ in the order $\tilde{\epsilon}^2$). In performing the integrals over the various combinations of powers of $\tilde{\epsilon}$, which occur after this expansion in the numerator and the denominator of Eq. (23), use can be made of the linked-cluster theorem. $G^{\text{1-hole}}$ contains spatially diagonal, h^{aa} and h^{bb} , as well as spatially off-diagonal terms, h^{ab} and h^{ba} . The latter are of the order of $\epsilon \sim 1/S^{1/2}$. Since they are proportional to the hopping integral t (cf. Eq. (19)), our expansion in $1/S$ becomes necessarily also an expansion in t . We shall neglect terms of order higher than t^2 .

The actual expansion is straight-forward but rather tedious. We express the result as

$$G(\tau) = e^{-\tilde{\tau}/2} \left(1 - \frac{1}{S} G^{(1)}(\tilde{\tau}) - \frac{1}{S^2} G^{(2)}(\tilde{\tau}) + \mathcal{O}\left(\frac{1}{S^3}\right) \right) . \quad (\text{B5})$$

For the first order coefficient, we obtain

$$G^{(1)}(\tilde{\tau}) = - \cdots \tilde{\tau} + \frac{1}{N} \sum_{\mathbf{k}} \frac{1 - e^{-\omega_{\mathbf{k}}\tilde{\tau}}}{4\omega_{\mathbf{k}}} (1 + \frac{4t^2}{dJ^2}) . \quad (\text{B6})$$

The first term in Eq. (B6), proportional to $\tilde{\tau}$, belongs to the expansion of $E_{\mathbf{q}}(S)$ in Eq. (25) and will consequently be neglected. In the evaluation of the momentum sum in the second term in Eq. (B6), we consider a finite lattice of N lattice points of the A-sublattice and exclude the point $\mathbf{k} = 0$ from the sum, since the corresponding mode is a Goldstone mode, the uniform rotation of all spins. Then, this term has a finite limit as $\tau \rightarrow \infty$ and defines $Z^{(1)}$, the first order correction of the quasi-particle weight in Eq. (26) as

$$Z^{(1)} = \frac{1}{N} \sum_{\mathbf{k} \neq 0} \frac{1}{4\omega_{\mathbf{k}}} (1 + \frac{4t^2}{dJ^2}) . \quad (\text{B7})$$

The calculation of the next order coefficient, $G^{(2)}(\tilde{\tau})$, proceeds exactly in the same way, but it is much more tedious. We neglect polynomial terms $\tilde{\tau}, \tilde{\tau}^2$, since they belong to the expansion of $E_{\mathbf{q}}(S)$ in Eq. (25), exclude the point $\mathbf{k} = 0$ from the momentum sums, and take the limit $\tau \rightarrow \infty$. Then finally, collecting all terms, we get the following result for the second order correction in the quasi-particle weight

$$Z^{(2)} = \frac{1}{N^2} \sum_{\substack{\mathbf{k} \neq 0 \\ \mathbf{k}' \neq 0}} \frac{1}{4\omega_{\mathbf{k}}} \frac{1}{4\omega_{\mathbf{k}'}} \left(A_{\mathbf{k},\mathbf{k}'} + \frac{4t^2}{dJ^2} B_{\mathbf{k},\mathbf{k}'} \right) , \quad (\text{B8})$$

with

$$A_{\mathbf{k},\mathbf{k}'} = \frac{1}{4} - \frac{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}{\omega_{\mathbf{k}} + \omega_{\mathbf{k}'}} , \quad (\text{B9})$$

$$\begin{aligned} B_{\mathbf{k},\mathbf{k}'} = & -1 + \frac{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}{(\omega_{\mathbf{k}} + \omega_{\mathbf{k}'})^2} \\ & + (\omega_{\mathbf{k}} + \omega_{\mathbf{k}'}) \left(\frac{3}{4} + \left[\frac{\gamma_{\mathbf{k}+\mathbf{k}'} - \gamma_{\mathbf{k}}\gamma_{\mathbf{k}'}}{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}} \right]^2 \right) \\ & - \frac{1}{2} \frac{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}}{\omega_{\mathbf{k}} + \omega_{\mathbf{k}'}} \left(3 + \left[\frac{\gamma_{\mathbf{k}+\mathbf{k}'} - \gamma_{\mathbf{k}}\gamma_{\mathbf{k}'}}{\omega_{\mathbf{k}}\omega_{\mathbf{k}'}} \right]^2 \right) \end{aligned} \quad (\text{B10})$$

In the preceding expressions for $A_{\mathbf{k},\mathbf{k}'}$ and $B_{\mathbf{k},\mathbf{k}'}$, we have neglected terms of order k^2 , k'^2 , or $\mathbf{k}\mathbf{k}'$ and higher.

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